

# High-precision scale setting in lattice QCD

## Budapest-Marseille-Wuppertal collaboration

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**ABSTRACT:** Scale setting is of central importance in lattice QCD. It is required to predict dimensional quantities in physical units. Moreover, it determines the relative lattice spacings of computations performed at different values of the bare coupling, and this is needed for extrapolating results into the continuum. Thus, we calculate a new quantity,  $w_0$ , for setting the scale in lattice QCD, which is based on the Wilson flow like the scale  $t_0$  (M. Luscher, JHEP 1008 (2010) 071). It is cheap and straightforward to implement and compute. In particular, it does not involve the delicate fitting of correlation functions at asymptotic times. It typically can be determined on the few per-mil level. We compute its continuum extrapolated value in  $2 + 1$ -flavor QCD for physical and non-physical pion and kaon masses, to allow for mass-independent scale setting even away from the physical mass point. We demonstrate its robustness by computing it with two very different actions (one of them with staggered, the other with Wilson fermions) and by showing that the results agree for physical quark masses in the continuum limit.

**KEYWORDS:** Lattice QCD, scale setting

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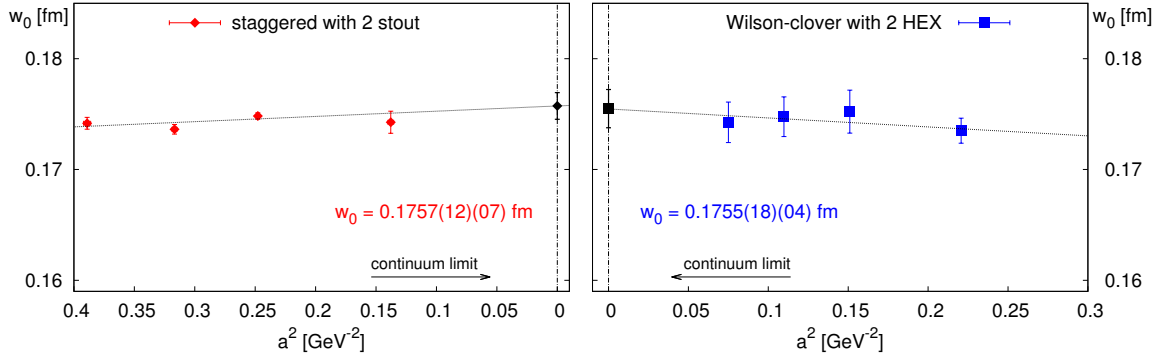
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## 1 Introduction

Quantum chromodynamics (QCD) is a theory with few parameters: the quark masses and an overall scale. To determine the latter, one has to compute a dimensionful quantity or an observable at a known energy, and adjust the overall scale of the theory to reproduce the corresponding experimental measurement. In lattice calculations this is equivalent to fixing the lattice spacing  $a$ . The lattice spacing is determined by calculating a dimensionful quantity  $Q$  –for definiteness,  $Q$  is chosen to be of mass dimension one here– such as the mass of the Omega baryon,  $M_\Omega$ , or the pion decay constant,  $F_\pi$ , and by relating its lattice value to its experimental value through  $a = (aQ)^{latt}/Q^{expt}$ . In principle any dimensionful



**Figure 1.** Representative continuum extrapolations of the  $w_0$  scale, at the physical mass point. The values at different lattice spacings are obtained by using the Wilson flow described below. The continuum limit values on the plots are results from our final, full analyses. The results obtained with the two very different actions (staggered fermions on the left and Wilson fermions on the right panel) are in good agreement and the overall uncertainties are very small.

quantity can be used. However, it is clear that the quality of any dimensionful prediction from the lattice can only be as good as the quality of the determination of the overall scale. This statement is particularly relevant now that lattice QCD results with errors below 2% are beginning to be reported.

Besides the overall scale in physical units, it is also important to accurately determine the relative lattice spacings of simulations performed at different values of the bare coupling in order to carry out a continuum extrapolation. Independent calculations can be compared too, if dimensionful quantities are expressed in units of a well measured quantity. For this purpose it may be useful to consider an observable which is not directly measured in experiment, but which is particularly simple to compute with high accuracy. Moreover, if this observable is computed accurately in physical units once, its value can be used in all subsequent lattice calculations to fix their overall scales.

One popular observable of this type is the Sommer scale,  $r_0$ , introduced nearly two decades ago [1]. More recently, MILC has found it more convenient to consider the related scale  $r_1$  [2]. One of the advantages of these scales is that they are based on the calculation of the static potential from gauge fields: they do not require the costly computation of quark propagators, as do observables such as  $M_\Omega$  or  $F_\pi$ . However, the determination of the potential requires a delicate study of the asymptotic time behavior of Wilson loops and the calculation of  $r_0$  or  $r_1$  from the potential is a much more complicated analysis (see [3] for a recent example) than, say, fitting the mass of a particle, such as the pion, from a measured correlator. The introduction of HYP smearing [4] on the gauge links has reduced the problem of the poor signal-to-noise ratio of Wilson loops, but the calculation of  $r_0$  or  $r_1$  remains non-trivial. These subtleties might be at least partially responsible for the tension within present determinations of the Sommer scale between [5] and [6, 7], and for a similar tension between recent and present determinations [7, 8]. While these differences are only on the two standard deviation level they have an important impact on the search for new physics in the leptonic decays of the  $D_s$  meson, as discussed in [9].

In this paper we propose an alternative to the  $r_0$  scale: the  $w_0$  scale. The method is based on the Wilson flow. The Wilson flow was considered in the context of trivializing maps by Luscher [10]. It was studied earlier by Narayanan and Neuberger [11] in a different context, too. Its important renormalization properties were clarified in [12, 13]. Its application to scale setting, which we build upon, was suggested recently in [12].

The  $w_0$  scale keeps the advantages of the Sommer scale (i.e. no expensive fermion inversion is needed). However, it is easier to determine with high precision, since it requires neither a fitting of the asymptotic time behavior of correlation functions nor fighting signal-to-noise issues.

Before discussing the method in detail (see Section 2), we present our results for the  $w_0$  scale in physical units. These values can henceforth be used to determine the lattice spacing in physical units in  $N_f = 2 + 1$  lattice QCD calculations. (The dependence of  $w_0$  on  $N_f$  should be studied before it is used to set the scale in simulations with  $N_f \neq 2 + 1$ .) We performed two independent calculations of  $w_0$ , both based on simulations with pion masses all the way down to its physical value and below. The first uses our 2HEX smeared Wilson fermion ensembles [14–16] and the second, 2-stout smeared staggered simulations [17–23].

In both cases  $w_0$  is interpolated to the physical quark masses as well as extrapolated into the continuum. The  $\Omega$  mass is used to convert these scales to physical units (with our smeared actions hadron mass ratios show very small cutoff effects [24, 25]). Representative continuum limits (see below) are displayed in Fig. 1, where the staggered and Wilson results are shown on the l.h.s. and r.h.s., respectively. The plot indicates that  $w_0$  has cutoff effects similar to  $M_\Omega$ , resulting in a very mild continuum scaling, and that the uncertainties on the extrapolated value are very small. Moreover, the staggered and Wilson results are in good agreement and the precisions reached with the two actions are on the same level. We quote the Wilson result, which does not rely on the “rooting” of the fermion determinant, as our final result:

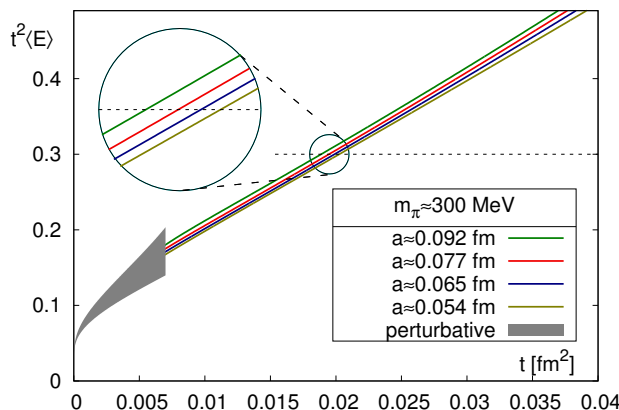
$$w_0 = 0.1755(18)(04) \text{ fm} , \quad (1.1)$$

where the first error is statistical and the second is systematic. Note that the overall uncertainty is 1%, most of which is statistical. Furthermore, the statistical error in the dimensionless quantity  $w_0 M_\Omega$  comes dominantly from  $aM_\Omega$ . Thus, the error on  $w_0/a$  itself is subdominant, typically on the level of a few per mil or less. This fact makes  $w_0/a$  a particularly attractive candidate to set the relative scale between simulations for continuum extrapolations and for comparing calculations from different groups. Another interesting application is the determination of the ratio of the lattice spacings for anisotropic actions [26]. As a side product we also compute a related quantity  $(t_0)^{1/2}$  suggested in [12] (though on the same set of configurations its *relative* systematic error is four times larger than that of  $w_0$ ).

This paper is organized as follows. After this introductory section we discuss the scale setting method based on the Wilson (and Symanzik) flow in Section 2. The next two sections (3,4) deal with our results obtained with Wilson and with staggered fermions, respectively. Section 5 discusses two possible problems, namely finite volume effects and autocorrelations for the flow. Section 6 presents the final results and concludes. In order to make the practical application of the scale setting procedure presented here easier, the method is implemented in the CHROMA software system [27]. In addition, along with this paper we submit two codes to the arXiv, both written in C, as ancillary files. The first (`wilson_flow.c`) determines the Wilson (and Symanzik) flow. It was written emphasizing readability over speed. It works both for isotropic and anisotropic [26] lattice actions. The second one (`w0_scale.c`) uses the output of `wilson_flow.c` or that of CHROMA to determine the scale  $w_0/a$  and its statistical uncertainty.

## 2 The scales $(t_0)^{1/2}$ and $w_0$

The scale setting method can be summarized as follows. Following the strategy of Ref. [12] we calculate the Wilson flow, that is we integrate infinitesimal gauge-field smearing steps up to a scale  $t$ , whose units are inverse mass-squared. The smearing is performed until a well-chosen dimensionless observable reaches a specified value. The universal “flow time,”  $t = t_0$ , at which this happens can then be used to set the scale on the original lattices.



**Figure 2.** Analogously to the Wilson flow in Fig. 2 of [12] here we show the Symanzik flow, which can be used to define the  $w_0$  scale and the  $t_0^{1/2}$  scale proposed by [12]. These flows are obtained using our  $N_f=2+1$  Wilson fermion simulations. For our four lattice spacings we have runs close to  $M_\pi \approx 300$  MeV (the individual pion masses are somewhat different). The perturbative expectation is shown by the gray band. Its width indicates the uncertainty in  $\Lambda_{QCD}$  using two representative values from the literature (c.f. Refs. [28, 29]).

Integrating the infinitesimal smearing steps is equivalent to finding the solution to the flow equation [11, 12]:

$$\dot{V}_t = Z(V_t)V_t, \quad V_0 = U \quad (2.1)$$

where  $V_t$  are the gauge links at flow time  $t$  and  $U$  are the original gauge links. In [12, 13], where the Wilson action is used,  $Z(V_t)$  is the derivative of the plaquette action and the corresponding flow is called the Wilson flow. As it can be seen from Eq. (2.1) an infinitesimal change of the link variable is obtained by the product of the link variable itself and the sum of the staples around it. Thus, for the present case the flow is generated by infinitesimal stout-smearing steps. As a consequence the action decreases and the gauge field is getting smoother. For improved gauge actions, one can take  $Z(V_t)$  to be the algebra-valued derivative of the gauge action.

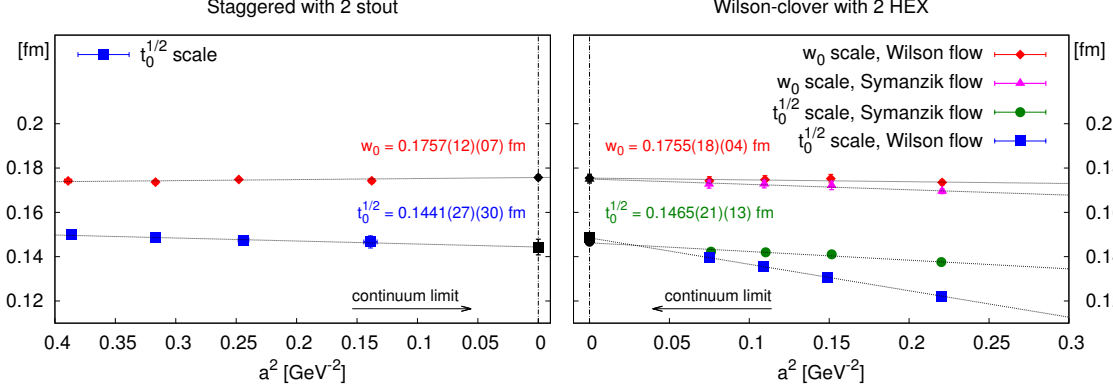
To obtain the scale  $t_0$ , it is suggested in [12] to integrate the flow and to compute  $t^2\langle E(t) \rangle$  as a function of  $t$ ,  $t_0$  being the flow time where  $t^2\langle E(t) \rangle$  reaches 0.3. Here  $\langle E(t) \rangle$  is the expectation value of the continuum-like action density  $G_{\mu\nu}^a(t)G_{\mu\nu}^a(t)/4$ , where  $G_{\mu\nu}^a(t)$  is a lattice version of the chromoelectric field-strength tensor at flow time  $t$ . Here we use the usual clover-leaf definition for this tensor. Note that  $t^2\langle E \rangle$  turned out to be approximately proportional to  $t$  for large flow times, a similar observation was made for the pure gauge theory in Ref. [12].

Here we propose to use another, related observable, namely

$$W(t) \equiv t \frac{d}{dt} \{t^2\langle E(t) \rangle\} \quad (2.2)$$

and define the  $w_0$  scale, via the condition

$$W(t)|_{t=w_0^2} = 0.3. \quad (2.3)$$



**Figure 3.** Representative continuum extrapolations of two different scale observables ( $t_0^{1/2}$  and  $w_0$ ) at physical quark masses, using our  $N_f = 2 + 1$  staggered (left panel) and Wilson (right panel) simulation data. An illustration of the different cutoff effects is also shown. We determined  $t_0^{1/2}$  and  $w_0$  with Wilson fermions using two different flow equations (Wilson and Symanzik flow). The results based on the different flow equations show different discretization effects. For the two very different actions the final results are in good agreement and the overall uncertainties on the continuum values are very small.

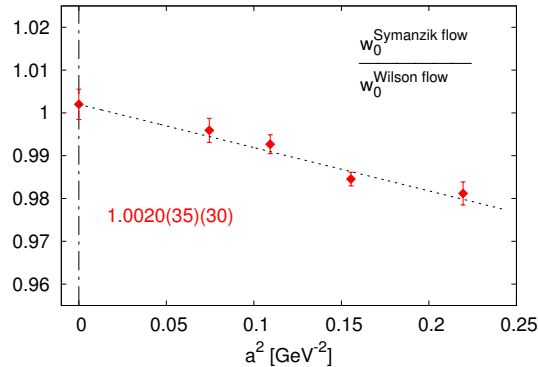
The most important reasons for this choice can be summarized as follows. While  $t^2\langle E(t) \rangle$  incorporates information about the gauge configurations from all scales larger than  $\mathcal{O}(1/\sqrt{t})$  (thus including scales also around the cutoff),  $W(t)$  mostly depends on scales around  $\mathcal{O}(1/\sqrt{t})$ . This is an advantage, because the behavior of the flow at small  $t \sim a^2$  is subject to discretization effects. Let us illustrate these cutoff effects by one example. The flow  $t^2\langle E(t) \rangle$  starts vertically at the origin in the continuum, while it must start horizontally for any lattice spacing and for any lattice action. The value of  $t^2\langle E(t) \rangle$  at  $t$  is influenced by this cutoff effect appearing at small  $t$ , whereas the derivative  $W(t)$  is less affected. In the original approach, the flow times  $t$  corresponding to different values of  $t^2\langle E(t) \rangle$  yield different relative scales. Contrary to that,  $W(t)$  yields very similar scales when different values are considered on the r.h.s. of (2.2). Furthermore, the perturbative calculation of [12] provides strong evidence that  $t_0$ , and also  $w_0$ , does not require renormalization.

Of course one is free to modify the lattice observable used or the flow equation (2.1) by terms which vanish in the continuum limit. For instance, as Section 3 of [12] discusses,  $\langle E(t) \rangle$  can be obtained directly from the sum of the plaquettes or from the more symmetric clover definition of  $G_{\mu\nu}^a(t)$ . Both definitions are acceptable and lead to results which must converge to the same continuum limit. One can look at the pure  $SU(3)$  gauge theory with no quarks and study the flow in units of  $r_0$ . The symmetric definition turns out to be advantageous [12], since it results in negligible cutoff effects, whereas the non-symmetric definition leads to approximately 5% cutoff effects at a lattice spacing of 0.1 fm [12]. The choice of  $Z(V_t)$  in (2.1) is also only fixed up to discretization corrections. The natural choice is to consider the algebra-valued derivative of the gauge action used in the simulation (cf. Section 6 of [10]). In our case this is a tree-level Symanzik improved action [30] and we call

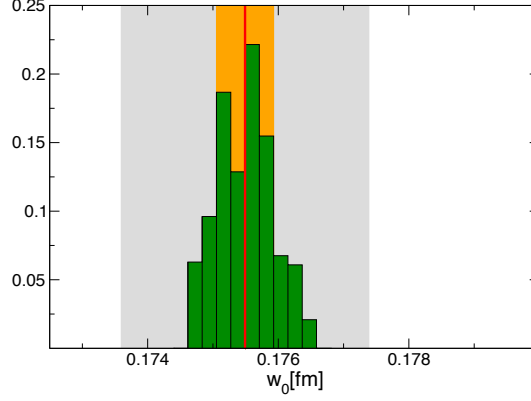
the corresponding flow, the Symanzik flow (c.f. Fig. 2). However, the use of the Wilson flow is also correct and should give the same continuum limit. This is illustrated in Fig. 3, with 2HEX Wilson fermions. As can be seen,  $t_0^{1/2}$  obtained by the Wilson flow has larger cutoff effects than the one coming from the Symanzik flow. For  $w_0$ , both choices are good and cutoff effects are around or less than two percent, in the range of lattice spacings considered. This is confirmed by looking at the ratio of the  $w_0$  scales obtained from the Symanzik and the Wilson flows as a function of lattice spacing. Fig. 4 shows that the ratio approaches 1 in the continuum limit, as it should. Here the pion and kaon masses are tuned to their physical values (this tuning leads to systematic uncertainties included on the points and discussed below). For our staggered action both  $t_0^{1/2}$  and  $w_0$  can be obtained with small cutoff effects using the Wilson flow. Note that in our case it is consistent to use one action for generating the fields and another one in the gauge flow. The two actions differ only in higher order in the lattice spacing, thus the derivative of the action with respect to the link variable will have the same order cutoff effect. Since in our setup the fermionic sector has already  $a^2$  cutoff effects –at least–, using the Wilson flow instead of the Symanzik flow does not deteriorate the continuum extrapolation. Obviously, one should use the same definition for different lattice spacings, if a continuum extrapolation is carried out.

In fact the  $w_0$  scale determined with the Wilson flow has tiny cutoff effects for both our Wilson and staggered actions. Since integrating the Wilson flow is several times faster than working with the Symanzik flow, the former provides a quick and straightforward determination of the lattice spacing through the  $w_0$  scale.

On a practical level, the flow equation (2.1) can be efficiently integrated by using the explicit fourth-order Runge-Kutta scheme proposed in [12]. The links at flow time  $t + \epsilon$



**Figure 4.** Ratio of the  $w_0$  scales obtained by Symanzik and Wilson flows for physical pion and kaon masses.



**Figure 5.** Final histogram for the different analyses used to compute  $w_0$  with our Wilson fermion simulations. Each entry is weighted by its corresponding fit quality. The orange (thinner) band denotes the systematic and the gray (thicker) one the combined (systematic and statistical) uncertainties. The vertical line depicts the central value. Due to the small width of the distribution (note the scale), our final result (1.1) is very precise.

are obtained from those at flow time  $t$  via

$$\begin{aligned}
X_0 &= V_t, \\
X_1 &= \exp\left(\frac{1}{4}Z_0\right) X_0, \\
X_2 &= \exp\left(\frac{8}{9}Z_1 - \frac{17}{36}Z_0\right) X_1, \\
V_{t+\epsilon} &= \exp\left(\frac{3}{4}Z_2 - \frac{8}{9}Z_1 + \frac{17}{36}Z_0\right) X_2,
\end{aligned} \tag{2.4}$$

where  $Z_i \equiv \epsilon Z(X_i)$ . It turns out that the step size  $\epsilon$  can be chosen rather coarse, since the total integration error associated with the finite step size scales like  $\epsilon^3$  [12]. Indeed we find that a value of  $\epsilon = 0.01$  yields finite-step-size errors far below the per-mil level, which is negligible for our purposes. These findings are in agreement with those of [12].

### 3 $N_f = 2 + 1$ Wilson fermion computation

We compute the  $w_0$  scale (and also the  $t_0^{1/2}$  scale) using our 2HEX smeared [31] Wilson fermion ensembles [14–16], dropping the coarsest lattice with  $\beta = 3.31$ , as it appears to be less suited for studying various options for flows and/or scale setting procedures. Note that we are still left with four lattice spacings, which provide a safe continuum extrapolation, and pion masses down to, or even below, the physical value.

As discussed above, the Symanzik or the Wilson flows are equally valid for determining scale observables. Our continuum results for these observables agree within systematic errors. In order to reduce the uncertainties coming from the continuum extrapolation, one should favor the flow which has small cutoff effects. As we illustrated in Fig. 3 the continuum extrapolation of the  $w_0$  scale with the Symanzik and the Wilson flows are almost



equally good (the Wilson flow is slightly better). For the  $t_0^{1/2}$  scale the Symanzik flow gives smaller cutoff effects than the Wilson flow, resulting in a factor of two smaller systematic error. Thus, for our results (c.f. Fig. 3) we used the flows with the smaller cutoff effects. Even with this favourable choice the *relative* systematic error of the  $t_0^{1/2}$  scale is still about four times larger than that of the  $w_0$  scale. This huge difference in accuracy justifies our preference for the  $w_0$  scale (for the  $w_0$  scale Symanzik or Wilson flows are similarly good). Moreover, since integrating the Wilson flow is several times faster than integrating the Symanzik flow, the best way to set the scale is to use  $w_0$  determined from the Wilson flow.

As discussed above, we use the  $\Omega$  baryon mass to express  $w_0$  in physical units. Thus, the scale is extracted from  $aM_\Omega$  at the point where the ratios  $(M_\pi/M_\Omega, M_K/M_\Omega)$  acquire their physical values, as described in [14]. We then compute  $w_0(M_\pi, M_K, a)$  in physical units for each ensemble and perform a combined quark-mass interpolation and continuum extrapolation to obtain the physical value of  $w_0$ .

Four different fit functions are used to interpolate to the physical mass point in the  $M_\pi$ – $M_K$  plane. They have the form  $w_0 = a_0 + a_1 M_\pi^2 + a_2 M_K^2 + d(a) + \text{hoc.}$ , where *hoc.* stands for higher order contributions in  $M_\pi^2$  and/or  $M_K^2$ . Because our fermion action is tree-level improved, the discretization corrections,  $d(a)$ , are chosen to be either proportional to  $\alpha_s a$  or  $a^2$  (since the continuum extrapolation of  $w_0/M_\Omega$  is practically constant, essentially no difference is observed between these two choices).

The various strategies that we apply for the mass extractions, to interpolate to the physical point and to extrapolate to the continuum limit are all combined to estimate the systematic uncertainties. To that end we use 64 different analyses, i.e. the 4 different fit forms in the  $M_\pi$ – $M_K$  plane, 2 pion mass cuts for these fits ( $M_\pi < 300$  MeV, 350 MeV), 2 different scaling assumptions in the lattice spacings, 2 fit ranges for extracting  $M_K$ ,  $M_\pi$  and  $M_\Omega$  as well as 2 methods for setting the scale (corresponding to different pion mass cuts in the  $M_\Omega$ -fits, i.e.  $M_\pi < 380$  MeV, 480 MeV). Each of these analyses can be fully justified

and can be considered “the” final analysis. Thus, according to our standard procedure [14, 16, 25, 32], we construct a histogram out of the values obtained for  $w_0$ , where each one is weighted by the corresponding fit quality. We compute the median and the central 68% confidence interval of the resulting distribution and take these values to be our central value and systematic error, respectively (cf. Fig. 5). A detailed error budget is given in Tab. 1. The same set of analyses has been repeated for the observable based on the Symanzik flow. We found an agreement within error (see Fig. 3).

source	relative error [%]
physical point interpolation	15
$M_\pi$ -cut	40
continuum limit	55
spectrum	55
scale	45

**Table 1.** Contributions to the systematic uncertainty on  $w_0$ , as fractions of the total systematic error in % (rounded to the closest 5%). The various uncertainties are explained in the main text and they are listed in the same order here. Note that the fractions must be added in quadrature and do not sum up exactly to 100% due to correlations and rounding.

$\beta$ , scale	$am_s$	$m_s/m_u$
3.7500	0.050254	28,14,10
$a^{-1} = 1.605(6)(3)$ GeV	0.048	27.9,20,10
	0.040	10
3.7920	0.05	20
$a^{-1} = 1.778(7)(1)$ GeV	0.045	28,20,14,10
	0.040	20,10
3.8500	0.0395	27.3,20,14,10
$a^{-1} = 2.024(18)(7)$ GeV	0.0388	20,14,10
	0.037	10
3.9900	0.0283	28.15,10,6
$a^{-1} = 2.684(58)(7)$ GeV	0.0277	14,10,6

**Table 2.** Staggered ensembles used in this analysis.

The statistical error is computed by repeating the analysis on 2000 bootstrap samples. Note that the statistical error is much larger than the systematic. The statistical error of  $w_0/a$  is much smaller than that of  $aM_\Omega$ . Therefore, the error of our  $w_0$  in physical units is dominated by the statistical uncertainties in  $aM_\Omega$ . In that way, we obtain the result with its systematic and statistical errors given in Eq. (1.1).

#### 4 $N_f = 2 + 1$ staggered fermion computation

An interesting test is a comparison of continuum results obtained with Wilson and staggered fermions. Therefore, we perform a fully independent determination of  $w_0$ . We consider the 2-step stout-smeared staggered fermion action [33] used in our thermodynamics studies [17–21, 34]. The parameters of the ensembles used here are summarized in Tab. 2. Note that the pion masses either straddle the physical value (obtained from  $M_\pi/M_\Omega$ ) or even touch it within errors. We express all quantities as functions of the bare masses for fixed gauge coupling. The  $w_0$  scale in lattice units,  $w_0/a(am_{ud}, am_s)$ , is then computed for each simulation point as described before. These results are then interpolated to the physical point. This interpolation is done for every lattice spacing separately. Again, we use four functional forms as in the Wilson case. Since there is no additive mass renormalization for staggered fermions and the bare quark masses are known exactly, in the interpolating fits we use these masses. Thus, instead of  $M_\pi^2$  we use  $2m_{ud}$  and instead of  $M_K^2$  we use  $m_{ud} + m_s$  in the fit functions. For both the kaon and pion mass, we use three polynomial fit formulae to describe their quark mass dependence. Finally, we perform a linear continuum extrapolation in  $a^2$ . In order to estimate the cutoff effects we use the four or the three finest lattice spacings. We end up with 72 different continuum values for  $w_0$ , where each one can be weighted by the combined goodness of fit. Note that we have a much larger statistics for our staggered action than for the Wilson one.

On a subset of the ensembles used here we have already carried out a scaling study for  $r_0$  in Ref. [19]. We found that for the same action and lattice spacing range one observes about 10% cutoff effect for  $r_0$  (see the right panel of Fig. 4 in Ref. [19], where the scale was set by  $f_K$ ). We also gave a scaling plot for  $M_\Omega$  in the same paper.

## 5 Finite volume effects and autocorrelations

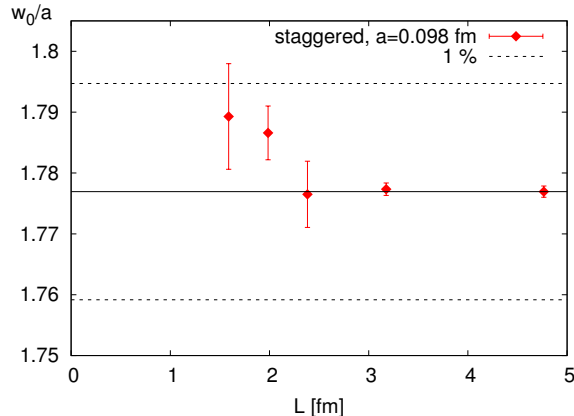
At fixed physical volume, finite-volume effects on the Wilson or Symanzik flow increase as the flow time increases. It is, therefore, important to check that these effects remain small for our choice of  $w_0$  scale. Fig. 6 displays the volume dependence of  $w_0/a$  on the second finest staggered lattice at physical quark masses. (For this test we used a couple of thousand trajectories for each volume.) It shows that finite-volume effects only become relevant for box sizes  $\lesssim 2$  fm. For lattices larger than that, finite volume effects are essentially absent. Note that for a lattice of 2 fm one has  $M_\pi L = 1.35$ , which is far smaller than the spatial size suggested by the rule of thumb  $M_\pi L \gtrsim 4$ . These tiny finite volume effects and the smallness of the error on  $w_0/a$  make the  $w_0$  scale a very attractive intermediate quantity to determine the lattice spacing.

Since the Wilson/Symanzik flow incorporates more and more information from the whole lattice as  $t$  increases, it is important to study autocorrelations. Thus, we compute the integrated autocorrelation time of the flow as a function of  $t$ , using the standard methodology described in [35]. We do so by looking at several long (5000 trajectories) parallel HMC streams on our finest staggered lattices or simply analyzing a long HMC stream on one of our finest Wilson ensembles [14]. We find that for lattice spacings down to about  $a = 0.054$  fm, the integrated autocorrelation time of  $E(t = w_0^2)$  is around or below 50 unit-length trajectories. These autocorrelations are taken into account by appropriate binning.

## 6 Results and conclusions

We presented a new quantity for setting the scale in lattice QCD calculations. Precise determinations of this new  $w_0$  scale were obtained using Wilson and staggered fermion simulations with lattice spacings down to 0.054 fm and average up and down quark masses all the way down to, and even below, its physical value. Therefore, we showed that the  $w_0$  scale can be used to reliably determine the lattice spacing in physical units in upcoming lattice calculations. Moreover, the good agreement between the Wilson and staggered determinations illustrates the robustness of this scale-setting method (c.f. Fig. 1).

In Eq. (2.2) we define the  $w_0$  scale as the square root of the “time” at which the logarithmic derivative of  $t^2 \langle E(t) \rangle$  reaches 0.3. A larger value, say 0.5, increases the cost of integrating the flow, as well as the size of statistical and finite-volume errors. A smaller value would probe short-distance physics which is more strongly affected by discretization errors. For values below 0.1, this becomes a serious concern for coarser lattices. The value 0.3 is chosen to be safely away from these two extremes and is optimal for modern day



**Figure 6.** Finite-volume effects in the  $w_0$  scale. Here we plot the measured values of  $w_0/a$  as a function of  $L$ , obtained with fixed bare quark masses corresponding to the physical point. Notice that it is perfectly feasible to determine  $w_0/a$  to per-mil precision on the 164 configurations we have on our  $48^3 \times 64$  lattice. Even for boxes of size slightly below 2 fm, deviations from the large-volume value never exceed 1%.

simulations, performed with lattice spacings in the range  $0.05 \text{ fm} \lesssim a \lesssim 0.1 \text{ fm}$  and lattice sizes larger than 2 fm.

The continuum extrapolated value of  $w_0$  for the physical point is given in Eq. (1.1):

$$w_0 = 0.1755(18)(04) \text{ fm}.$$

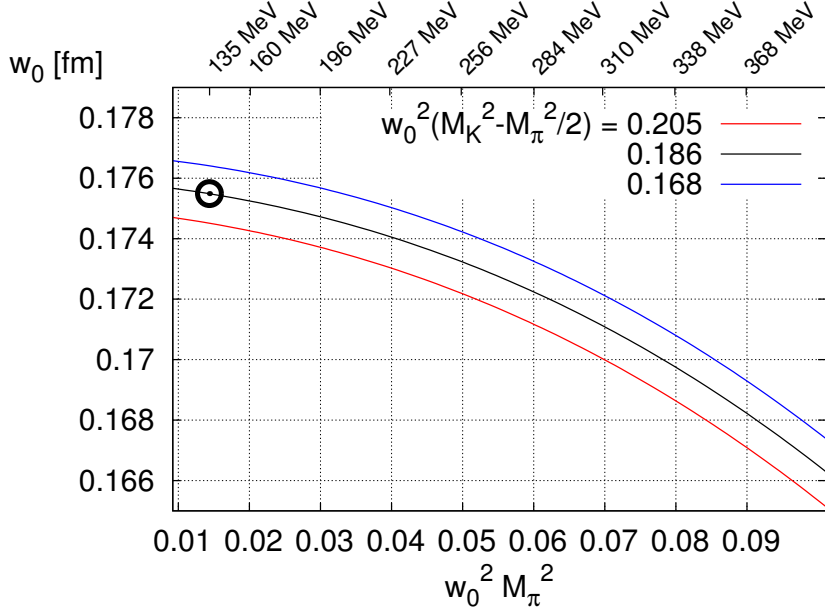
For non-physical pion and/or kaon masses the pion and kaon mass dependence of  $w_0$  is displayed in Fig. 7. This figure allows to determine the lattice spacing and its uncertainty as follows. One measures  $M_\pi a$ ,  $M_K a$  and  $w_0/a$ . Using these three quantities one then determines the dimensionless combinations  $x = w_0^2 M_\pi^2$  and  $y = w_0^2 (M_K^2 - M_\pi^2/2)$ . These two quantities define a point in Fig. 7. Reading off the value of  $w_0$  in physical units and combining it with the computed value of  $w_0/a$  gives the lattice spacing in fm. For pion and kaon masses covered by this figure the uncertainty of the  $w_0$  scale is essentially mass independent and its value is 1% (fully dominated by the statistical error of  $M_\Omega$ ). The same result for  $w_0$  and the lattice spacing can be obtained by using the following formula:

$$w_0 = 0.18515 - 0.5885x^2 - 0.0497y - 0.11xy - 1.476x^3 \pm 18 \cdot 10^{-3}(\text{stat}) \pm 4 \cdot 10^{-3}(\text{sys}) \quad (6.1)$$

which is valid for  $0.01 \lesssim x \lesssim 0.1$  and  $0.165 \lesssim y \lesssim 0.205$ .

In this paper we have shown that the  $w_0$  scale has several advantages over other scale setting procedures (most of which are also shared by  $t_0$ , though the latter is more sensitive to cut-off effects). The most important are:

- $w_0$  is cheap and easy to implement and compute (note that our reference implementations are publicly available); in particular:
  - $w_0$  does not require the computation of quark propagators;



**Figure 7.** The value of the  $w_0$  scale at various pion and kaon masses in the continuum limit. The results are based on our Wilson simulations. The black dot represents the physical point. To use the figures one should compute  $aM_\pi$ ,  $aM_K$  and  $w_0/a$ . Then one reads off the value of  $w_0$  in physical units corresponding to the combinations  $w_0^2 M_\pi^2$  and  $w_0^2 (M_K^2 - M_\pi^2/2)$ . The black curve in the middle corresponds to the physical  $M_K^2 - M_\pi^2/2$  (used to fix  $m_s$ ), whereas the lines below/above correspond to a 10% smaller/larger value of this quantity. As it can be seen the change in  $w_0$  is small. Changing the pion mass from its physical value to a three times larger value (thus, almost an order of magnitude larger quark mass) results in about 5% change in  $w_0$ . Changing the strange quark mass by 10% means changing  $w_0$  on the 0.5% level. The mass independent scale setting prescription is used here.

–  $w_0$  does not involve the delicate fitting of correlation functions at asymptotic times.

- the determination of  $w_0$  is not only cheap but it can be done precisely and reliably; typically one obtains results with an accuracy on the few per mil level;
- the value of  $w_0$  in physical units is known for physical and non-physical quark masses (for mass independent scale setting);
- our results suggest that  $w_0$  depends weakly on quark masses; in particular, unlike scale setting with  $M_\Omega$ , even a 10% deviation in  $m_s$  from its physical value only translates into a  $\lesssim 0.5\%$  change in the  $w_0$  scale;
- in the present investigation the most precise and fastest method to determine the scale was  $w_0$  based on the Wilson flow: independently of the type of the flow  $w_0$  has quite small cutoff effects and consequently small systematic uncertainties, whereas integrating the Wilson flow is the fastest among all flow choices.

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## References

- [1] R. Sommer, *A New way to set the energy scale in lattice gauge theories and its applications to the static force and alpha-s in SU(2) Yang-Mills theory*, *Nucl.Phys.* **B411** (1994) 839–854, [[hep-lat/9310022](#)].
- [2] C. W. Bernard, T. Burch, K. Orginos, D. Toussaint, T. A. DeGrand, et al., *The Static quark potential in three flavor QCD*, *Phys.Rev.* **D62** (2000) 034503, [[hep-lat/0002028](#)].
- [3] M. Donnellan, F. Knechtli, B. Leder, and R. Sommer, *Determination of the Static Potential with Dynamical Fermions*, *Nucl.Phys.* **B849** (2011) 45–63, [[arXiv:1012.3037](#)].
- [4] A. Hasenfratz and F. Knechtli, *Flavor symmetry and the static potential with hypercubic blocking*, *Phys.Rev.* **D64** (2001) 034504, [[hep-lat/0103029](#)].
- [5] **RBC Collaboration, UKQCD Collaboration**, Y. Aoki et al., *Continuum Limit Physics from 2+1 Flavor Domain Wall QCD*, *Phys.Rev.* **D83** (2011) 074508, [[arXiv:1011.0892](#)].
- [6] **HPQCD Collaboration**, C. Davies, E. Follana, I. Kendall, G. Lepage, and C. McNeile, *Precise determination of the lattice spacing in full lattice QCD*, *Phys.Rev.* **D81** (2010) 034506, [[arXiv:0910.1229](#)].
- [7] **Fermilab Lattice and MILC Collaborations**, A. Bazavov et al., *B- and D-meson decay constants from three-flavor lattice QCD*, [arXiv:1112.3051](#). 63 pages, 13 figures.
- [8] **HPQCD Collaboration, UKQCD Collaboration**, E. Follana, C. Davies, G. Lepage, and J. Shigemitsu, *High Precision determination of the pi, K, D and D(s) decay constants from lattice QCD*, *Phys.Rev.Lett.* **100** (2008) 062002, [[arXiv:0706.1726](#)].
- [9] A. S. Kronfeld, *The  $f_{D_s}$  Puzzle*, [arXiv:0912.0543](#).
- [10] M. Luscher, *Trivializing maps, the Wilson flow and the HMC algorithm*, *Commun.Math.Phys.* **293** (2010) 899–919, [[arXiv:0907.5491](#)].
- [11] R. Narayanan and H. Neuberger, *Infinite N phase transitions in continuum Wilson loop operators*, *JHEP* **0603** (2006) 064, [[hep-th/0601210](#)].
- [12] M. Luscher, *Properties and uses of the Wilson flow in lattice QCD*, *JHEP* **1008** (2010) 071, [[arXiv:1006.4518](#)].
- [13] M. Luscher and P. Weisz, *Perturbative analysis of the gradient flow in non-abelian gauge theories*, *JHEP* **1102** (2011) 051, [[arXiv:1101.0963](#)].
- [14] S. Durr, Z. Fodor, C. Hoelbling, S. Katz, S. Krieg, et al., *Lattice QCD at the physical point: Simulation and analysis details*, *JHEP* **1108** (2011) 148, [[arXiv:1011.2711](#)].
- [15] S. Durr, Z. Fodor, C. Hoelbling, S. Katz, S. Krieg, et al., *Lattice QCD at the physical point: light quark masses*, *Phys.Lett.* **B701** (2011) 265–268, [[arXiv:1011.2403](#)].
- [16] S. Durr, Z. Fodor, C. Hoelbling, S. Katz, S. Krieg, et al., *Precision computation of the kaon bag parameter*, *Phys.Lett.* **B705** (2011) 477–481, [[arXiv:1106.3230](#)].

- [17] Y. Aoki, G. Endrodi, Z. Fodor, S. Katz, and K. Szabo, *The Order of the quantum chromodynamics transition predicted by the standard model of particle physics*, *Nature* **443** (2006) 675–678, [[hep-lat/0611014](#)].
- [18] Y. Aoki, Z. Fodor, S. Katz, and K. Szabo, *The QCD transition temperature: Results with physical masses in the continuum limit*, *Phys.Lett.* **B643** (2006) 46–54, [[hep-lat/0609068](#)].
- [19] Y. Aoki, S. Borsanyi, S. Durr, Z. Fodor, S. D. Katz, et al., *The QCD transition temperature: results with physical masses in the continuum limit II.*, *JHEP* **0906** (2009) 088, [[arXiv:0903.4155](#)].
- [20] **Wuppertal-Budapest Collaboration**, S. Borsanyi et al., *Is there still any  $T_c$  mystery in lattice QCD? Results with physical masses in the continuum limit III*, *JHEP* **1009** (2010) 073, [[arXiv:1005.3508](#)].
- [21] S. Borsanyi, G. Endrodi, Z. Fodor, A. Jakovac, S. D. Katz, et al., *The QCD equation of state with dynamical quarks*, *JHEP* **1011** (2010) 077, [[arXiv:1007.2580](#)].
- [22] G. Endrodi, Z. Fodor, S. Katz, and K. Szabo, *The QCD phase diagram at nonzero quark density*, *JHEP* **1104** (2011) 001, [[arXiv:1102.1356](#)].
- [23] S. Borsanyi, Z. Fodor, S. D. Katz, S. Krieg, C. Ratti, et al., *Fluctuations of conserved charges at finite temperature from lattice QCD*, *JHEP* **1201** (2012) 138, [[arXiv:1112.4416](#)]. 13 pages, 8 figures in Jhep style.
- [24] S. Durr, Z. Fodor, C. Hoelbling, R. Hoffmann, S. Katz, et al., *Scaling study of dynamical smeared-link clover fermions*, *Phys.Rev.* **D79** (2009) 014501, [[arXiv:0802.2706](#)].
- [25] S. Durr, Z. Fodor, J. Frison, C. Hoelbling, R. Hoffmann, et al., *Ab-Initio Determination of Light Hadron Masses*, *Science* **322** (2008) 1224–1227, [[arXiv:0906.3599](#)].
- [26] S. Borsanyi et al., *Anisotropic lattices without tears*, *WUB/12-03* (2012).
- [27] **SciDAC Collaboration, LHPC Collaboration, UKQCD Collaboration**, R. G. Edwards and B. Joo, *The Chroma software system for lattice QCD*, *Nucl.Phys.Proc.Suppl.* **140** (2005) 832, [[hep-lat/0409003](#)].
- [28] E. Shintani, S. Aoki, H. Fukaya, S. Hashimoto, T. Kaneko, et al., *Strong coupling constant from vacuum polarization functions in three-flavor lattice QCD with dynamical overlap fermions*, *Phys.Rev.* **D82** (2010) 074505, [[arXiv:1002.0371](#)].
- [29] C. McNeile, C. Davies, E. Follana, K. Hornbostel, and G. Lepage, *High-Precision  $c$  and  $b$  Masses, and QCD Coupling from Current-Current Correlators in Lattice and Continuum QCD*, *Phys.Rev.* **D82** (2010) 034512, [[arXiv:1004.4285](#)].
- [30] M. Luscher and P. Weisz, *On-Shell Improved Lattice Gauge Theories*, *Commun.Math.Phys.* **97** (1985) 59.
- [31] S. Capitani, S. Durr, and C. Hoelbling, *Rationale for UV-filtered clover fermions*, *JHEP* **0611** (2006) 028, [[hep-lat/0607006](#)].
- [32] S. Durr, Z. Fodor, C. Hoelbling, S. Katz, S. Krieg, et al., *The ratio  $FK/F_{pi}$  in QCD*, *Phys.Rev.* **D81** (2010) 054507, [[arXiv:1001.4692](#)].
- [33] C. Morningstar and M. J. Peardon, *Analytic smearing of  $SU(3)$  link variables in lattice QCD*, *Phys.Rev.* **D69** (2004) 054501, [[hep-lat/0311018](#)].
- [34] S. Borsanyi, G. Endrodi, Z. Fodor, A. Jakovac, S. Katz, et al., *QCD equation of state from the lattice*, *AIP Conf.Proc.* **1343** (2011) 519–521.

- [35] **ALPHA collaboration**, U. Wolff, *Monte Carlo errors with less errors*, *Comput.Phys.Commun.* **156** (2004) 143–153, [[hep-lat/0306017](#)].
- [36] G. I. Egri, Z. Fodor, C. Hoelbling, S. D. Katz, D. Nogradi, et al., *Lattice QCD as a video game*, *Comput.Phys.Commun.* **177** (2007) 631–639, [[hep-lat/0611022](#)].